

**Computer and Computational Sciences Division
Publications and Presentations,
March 2004-March 2005**

Advanced Computing Laboratory (CCS-1)

Radiant Team

Book Chapter

W. Feng, “Green Destiny + mpiBLAST = Bioinformagic,” in *Advances in Parallel Computing* (series), *Parallel Computing: Software Technology, Algorithms, Architectures, and Applications*, Vol. 13, G.R. Joubert, W.E. Nagel, F.J. Peters, and W.V. Walter (editors), Elsevier. 2004.

Journal Publications

L. Carey, A. Darling, and W. Feng, “Takeoff with mpiBLAST: Parallel Searching,” *ClusterWorld Magazine*, Vol. 2, No. 3, March 2004.

M. Gardner, S. Thulasidasan, and W. Feng, “User-Space Auto-Tuning for TCP Flow Control in Computational Grids,” *Computer Communications, Special Issue on Network Support for Grid Computing*, 27(14): 1364-1374, September 2004.

J. Hurwitz and W. Feng, “Analyzing MPI Performance over 10-Gigabit Ethernet,” *Journal of Parallel and Distributed Computing, Special Issue: Design and Performance of Networks for Super-, Cluster-, and Grid-Computing*, 2005 (to appear).

C. Jin, D. Wei, S. Low, G. Buhrmaster, J. Bunn, D. Choe, R. Cottrell, J. Doyle, W. Feng, O. Martin, H. Newman, F. Paganini, S. Ravot, and S. Singh, “FAST TCP: From Theory to Experiments,” *IEEE Network*, January-February 2005.

M. Veeraraghavan, X. Zheng, W. Feng, H. Lee, E. Chong, and H. Li, “Scheduling and Transport for File Transfers on High-Speed Optical Circuits,” *Journal of Grid Computing*, 1(4): 395-405, June 2004.

X. Zhang, L. Bhuyan, and W. Feng, “Anatomy of UDP and M-VIA for Cluster Communication,” *Journal of Parallel and Distributed Computing, Special Issue: Design and Performance of Networks for Super-, Cluster-, and Grid-Computing*, 2005 (to appear).

Resilient Technologies

R. Aulwes, D. Daniel, N. Desai, R. Graham, L. Risinger, M. Sukalski, and M. Taylor, "Architecture of LA-MPI, a network-fault-tolerant MPI," in the *Proceedings of the 18th International Parallel and Distributed Processing Symposium*, Santa Fe, N.M., April 2004.

S. Ayyorgun and R. Cruz, "A Composable Service Model with Loss and a Scheduling Algorithm," in the *Proceedings of the 23rd IEEE Conference on Computer Communications (INFOCOM)*, Hong Kong, March 7-11, 2004. (Also a technical report, LA-UR-03-3939, Los Alamos National Laboratory.)

S. Ayyorgun and R. Cruz, "A Scheduling Problem in Interference-Limited Wireless Networks," in the *Proceedings of the 3rd IEEE International Conference on Networking (ICN)*, pp. 537-544, Guadeloupe, French Caribbean, March 1-March 4, 2004. (Also a technical report, LA-UR-03-7269, Los Alamos National Laboratory.)

S. Ayyorgun and R. Cruz, "A Service-Curve Model with Loss and a Multiplexing Problem," in the *Proceedings of the 24th IEEE International Conference on Distributed Computing Systems (ICDCS)*, pp. 756-765, Tokyo, Japan, March 23-26, 2004. (Also a technical report, LA-UR-03-3939, Los Alamos National Laboratory.)

S. Ayyorgun and R. Cruz, "Interference Control at Packet-Level in Wireless Networks with Quality-of-Service Support," in the *Proceedings of the 2nd IEEE Workshop on Modeling and Optimization in Mobile, Ad-Hoc, and Wireless Networks (WiOpt)*, pp. 20-29, Cambridge, U.K., March 24-26, 2004. (Also a technical report, LA-UR-03-8012, Los Alamos National Laboratory.)

S. Ayyorgun and W. Feng, "A Deterministic Characterization of Network Traffic for Average Performance Guarantees," in the *Proceedings of the 38th Annual Conference on Information Sciences and Systems (CISS)*, pp. 405-413, Princeton, N.J., March 17-19, 2004. (Also a technical report, LA-UR-03-4477, Los Alamos National Laboratory.)

S. Ayyorgun and W. Feng, "A Systematic Approach for Providing End-to-End Probabilistic QoS Guarantees," in the *Proceedings of the 13th IEEE International Conference on Computer Communications and Networks (ICCCN)*, pp. 115-122, Chicago, Ill., October 11-14, 2004. (Also two technical reports, LA-UR-03-3668 and LA-UR-03-7267, Los Alamos National Laboratory.)

A. Ayyorgun, S. Vanichpun, and W. Feng, "Probabilistic QoS Guarantees over Switches and Multiplexers," in the *Proceedings of the 42nd Annual Allerton Conference on Communication, Control, and Computing (ALLERTON)*, Monticello, Ill., September 29-October 1, 2004. (Also a technical report, LA-UR-03-7268, Los Alamos National Laboratory.)

S Ayyorgun, S. Vanichpun, and W. Feng, "Q-Composer and CpR: A Probabilistic Synthesizer and Regulator of Traffic (A Probabilistic Control of Buffer Occupancy)," in the *Proceedings of the 24th IEEE Conference on Computer Communications (INFOCOM)*, Miami, Fla., March 13-17, 2005. (Also a technical report, LA-UR-04-1270, Los Alamos National Laboratory.)

R. Castain, W. Saylor, and H.J. Siegel, "Application of Lagrangian Receding Horizon Techniques to Resource Management in Ad Hoc Grid Environments," 13th Heterogeneous Computing Workshop, in the *Proceedings of the 18th International Parallel and Distributed Processing Symposium*, Santa Fe, N.M., April 2004.

E. Gabriel, R. Graham, R. Castain, D. Daniel, T. Woodall, M. Sukalski, G. Fagg, E. Gabriel, G. Bosilca, T. Angskun, J. Dongarra, J. Squyres, V. Sahay, P. Kambadur, B. Barrett, and A. Lumsdaine, "Open MPI: Goals, Concept, and Design of a Next Generation MPI," in *Recent Advances in Parallel Virtual Machine and Message Passing Interface: 11th European PVM/MPI Users' Group Meeting*, Budapest, Hungary, September 19-22, 2004. Proceedings, Springer-Verlag, September 2004.

R. Graham, R. Castain, D. Daniel, T. Woodall, M. Sukalski, G. Fagg, E. Gabriel, G. Bosilca, T. Angskun, J. Dongarra, J. Squyres, V. Sahay, P. Kambadur, B. Barrett, and Andrew Lumsdaine, "TEG: A High-Performance, Scalable, Multi-Network Point-to-Point Communications Methodology," in the *Proceedings of the European PVM/MPI*, Springer-Verlag, September 2004.

J. Squyres, V. Sahay, P. Kambadur, B. Barrett, A. Lumsdaine, R. Castain, D. Daniel, R. Graham, T. Woodall, M. Sukalski, T. Angskun, G. Bosilca, G. Fagg, E. Gabriel, and J. Dongarra, "A Component Architecture of Message Passing Middleware," in *Cluster '04*, June 2004.

T. Woodall, R. Castain, D. Daniel, R. Graham, M. Sukalski, G. Fagg, E. Gabriel, G. Bosilca, T. Angskun, J. Dongarra, J. Squyres, V. Sahay, P. Kambadur, B. Barrett, and A. Lumsdaine, "Open MPI's TEG Point-to-Point Communications Methodology: Comparison to Existing Implementations," in the *European PVM/MPI*, Springer-Verlag, September 2004.

W. Yu, T. Wodall, R. Graham, and D. Panda, "Design and Implementation of Open MPI over Quadrics/Elan4," in the *19th International Parallel and Distributed Processing Symposium*, Denver, Colo., 2005.

Visualization

P. McCormick and J. Ahrens, "Large-Scale Data Visualization and Rendering—A Problem-Driven Approach," *Visualization Handbook*, Chris Johnson and Charles Hansen (editors), Academic Press, 2005.

P. McCormick, J. Inman, J. Ahrens, C. Hansen, and G. Roth, "Scout: A Hardware-Accelerated System for Quantitatively Driven Visualization and Analysis," IEEE Visualization 2004, pp. 171–178.

Software Components

A. Malony, S. Shende, N. Trebon, J. Ray, R. Armstrong, C. Rasmussen, and M. Sottile, "Performance Technology for Parallel and Distributed Component Software," *Concurrency and Computation: Practice and Experience*.

C. Rasmussen, M. Sottile, J. Nieplocha, R. Numrich, and E. Jones, "Co-Array Python: A Parallel Extension to the Python Language," *Euro-Par 2004 Parallel Processing*.

C. Rasmussen, M. Sottile, S. Shende, and A. Malony, "Bridging the Language Gap in Scientific Computing: The Chasm Approach," *Concurrency and Computation: Practice and Experience*.

C. Rickett, S. Choi, C. Rasmussen, and M. Sottile, "Rapid Prototyping Frameworks for Developing Scientific Applications: A Case Study," in *Proceedings of the Los Alamos Computer Science Institute Symposium (CDROM)*.

X. Zhao, J. Johnson, and C. Rasmussen, "Surface Tension of Quantum Fluids from Molecular Simulations," *Journal of Chemical Physics*.

Continuum Dynamics (CCS-2)

Telluride Team

B. Cooke, B. Smith, et al., "Modeling the MTI Electro-Optic System Sensitivity and Resolution," IEEE Transactions on Geoscience and Remote Sensing, in press.

J. Cullum, M. Hall, W. Joubert, T. Betlach, and B. Lally, "Scalable Parallel Linear Solvers for ASCI Applications—Scaling Across Thousands of Processors," technical report LA-UR-04-1879, Los Alamos National Laboratory. (Presentation to the CCS Division Review Committee.)

S. Cummins, M. Francois, D. Kothe, "Estimating Curvature from Volume Fractions, Computers and Structures," Vol. 83, Issue: 6-7, pp. 425-434, February 2005.

S. Cummins and D. Kothe, "A Study of Eulerian Phase Front Models for Crystal Growth," technical report, LA-UR-04-2390, Los Alamos National Laboratory.

S. Cummins, J. Mohd-Yusof, M. Francois, D. Kothe, "Eulerian Techniques for Crystal Growth," Telluride Workshop presentation, June 2004, and technical report, LA-UR-04-4250, Los Alamos National Laboratory.

A. Davis, M. Hall, and Igor N. Polonsky, “Three-Dimensional Radiative Transfer, Simplified ... with Cloud Modeling and Remote Sensing in Mind,” technical report, LA-UR-05-2282, Los Alamos National Laboratory. (Presentation to the ARM Science Team Meeting in Daytona Beach, Fla.)

M. Francois, “Interfacial Flow Computations with the Volume of Fluid and Immersed Boundary Methods,” presented at invited seminars at New Mexico State University, Texas A&M, and the University of Illinois at Urbana-Champaign. (Also a technical report, LA-UR-04-1852, Los Alamos National Laboratory.)

M. Francois, “Modeling of Surface Tension Force within a Volume-of-Fluid Formulation,” presented at a Los Alamos National Laboratory, CCS-2 seminar, June 2004. (Also a technical report, LA-UR-04-4207, Los Alamos National Laboratory.)

M. Francois, S. Cummins, E. Dendy, D. Kothe, J. Sicilian, and M. Williams, “A Balanced-Force Algorithm for Continuous and Sharp Interfacial Surface Tension Models within a Volume Tracking Framework,” technical report, LA-UR-05-0674, Los Alamos National Laboratory. (Also submitted to *Journal of Computational Physics*, 2005.)

M. Francois, E. Dendy, D. Kothe, J. Sicilian, M. Williams, and S. Cummins, “Improvements on the Modeling of Surface Tension in Truchas,” presented at the Truchas Workshop, Los Alamos, June 2004. (Also a technical paper, LA-UR-04-4103, Los Alamos National Laboratory.)

M. Francois, D. Kothe, S. Cummins, “Modeling Surface Tension Using a Ghost Fluid Technique within a Volume of Fluid Formulation,” in the Proceedings of the 21st International Congress on Theoretical and Applied Mechanics (ICTAM 04), Warsaw, Poland, August 2004. (Also a technical report, LA-UR-04-0413, Los Alamos National Laboratory.)

M. Hall and A. Davis, “Progress Toward Higher-Fidelity Yet Efficient Modeling of Radiation Energy Transport through Three-Dimensional Clouds,” technical report, LA-UR-05-2275, Los Alamos National Laboratory. (Also a presentation to the ARM Science Team Meeting in Daytona Beach, Fla.)

W. Joubert, M. Hall, J. Cullum, T. Betlach, and Bryan Lally, “Experiences with Linear Solvers on ASCI Applications: Achieving Scalability and Related Issues,” technical report, LA-UR-04-1462, Los Alamos National Laboratory. (Also a presentation to the ASCI Computational Physics Methods Workshop in Monterey, Calif.)

W. Joubert, M. Hall, J. Cullum, and B. Lally, “The LAMG Solver Library: Recent Results and Future Plans,” technical report, LA-UR-05-1345, Los Alamos National Laboratory. (Also a presentation at LANL.)

D. Lorstad, M. Francois, W. Shyy, and L. Fuchs, "Assessment of Volume of Fluid and Immersed Boundary Methods for Droplet Computations," *International Journal for Numerical Methods in Fluids*, Vol. 46, pp. 109-125, September 2004.

J. Turner, "Linear and Nonlinear Solvers in Truchas," technical report, LA-UR-04-4260, Los Alamos National Laboratory. (Also a presentation in June 2004 at the Second Annual Telluride Workshop.)

J. Turner and D. Kothe, "Implications of Petascale Computing for LANL Applications," technical report, LA-UR number pending, Los Alamos National Laboratory. (Also a presentation in March 2005 at the Department of Energy Office of Science Petascale/s Compact Simulation Application Workshop.)

J. Turner and S. Swaminarayan. "Radiative Heat Transfer in Truchas," technical report, LA-UR-04- 4329, Los Alamos National Laboratory. (Also a presentation in June 2004 at the Second Annual Telluride Workshop.)

Radiation Hydrodynamics Team

M. Christon, "Compatible Extensions for Finite Element Lagrangian Hydrodynamics," to be presented at the Eighth U.S. National Congress on Computational Mechanics, Austin, Texas, July 24-28, 2005. (Also a technical report, LA-UR-05-2032, Los Alamos National Laboratory.)

M. Christon and R. Patil, "A Finite Element Projection Method for Low-Mach Number Reacting Flows," to appear in Proceedings of the Third MIT Conference on Computational Fluid and Solid Mechanics, K.J. Bathe (editor), Elsevier, 2005. (Also a technical report, LA-UR-05-2031, Los Alamos National Laboratory.)

G. Dilts, "Consistent Thermodynamic Derivative Estimates for Tabular Equations of State," submitted to *Physical Review E*, March 2005.

G. Dilts, "Physically Realistic EOS Derivative Estimates," in the Proceedings of the Nuclear Explosives Code Developers Conference, Oct 4-7, 2004, Livermore, Calif.

D. Holm, C. Jeffery, S. Kurien, D. Livescu, M. Taylor, and B. Wingate, "The LANS-Alpha Model for Computing Turbulence: Origins, Results, and Open Problems," *Los Alamos Science* 29, 152-171, 2005.

K. Lipnikov, J. Morel, and M. Shashkov, "Mimetic Finite Difference Methods for Diffusion Equations on Non-Orthogonal Non-Conformal Meshes," *Journal of Computational Physics*, 199, 589-597, 2004.

D. Livescu, "Characteristics of Small Scale Turbulence in Homogeneous Turbulent Shear Flow," 57th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Seattle, Wash., November 23, 2004.

D. Livescu, "Comment on Compressible Rayleigh-Taylor Instabilities in Supernova Remnants (*Phys. of Fluids* 16, 4661, [2004])," to appear in *Physics of Fluids*, 2005.

D. Livescu, "Compressibility Effects on the Rayleigh-Taylor Instability," Turbulent Working Group Seminar, Los Alamos National Laboratory, July 7, 2004.

D. Livescu, "Compressibility Effects on the Rayleigh-Taylor Instability in the Linear and Weakly Nonlinear Stage," Turbulent Mixing Group Colloquium, Los Alamos National Laboratory, June 28, 2004.

D. Livescu, "Overview of the Compressible Rayleigh-Taylor Instability," LDRD-DR Seminar, Los Alamos National Laboratory, December 10, 2004.

D. Livescu, "Stochastic Large Eddy Simulations on Coarse Grids," LDRD-DR review, Los Alamos National Laboratory, March 22, 2004.

D. Livescu and C. Madnia, "Characteristics of Small Scale Turbulence in Homogeneous Turbulent Shear Flow," *Bulletin of American Physical Society* 49(10), 157, 2004. (Also presented at the 57th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Seattle, Wash., November 21-23, 2004.)

D. Livescu and C. Madnia, "Small Scale Structure of Homogeneous Turbulent Shear Flow," *Physics of Fluids* 16(8), 2864-2876, 2004.

R. Loubere and E. Caramana, "The Force/Work Differencing of Exceptional Points in the Discrete, Compatible Formulation of Lagrangian Hydrodynamics," technical report, LAUR-04-8906, Los Alamos National Laboratory.

J. Morel, B. Adams, Taewan Noh, J. McGhee, T. Evans, and T. Urbatsch, "Spatial Discretizations for Self-Adjoint Forms of the Radiative Transfer Equations," submitted to the *Journal of Computational Physics*.

J. Morel and J. Densmore, "A Two-Component Equilibrium Diffusion Limit," *Annals of Nuclear Energy*, 31, 2049-2057, 2004.

J. Morel and K. Lathrop, "Singular Solutions, Integral Transport Theory, and the Sn Method," *Nuclear Science and Engineering*, 147, 158-166, 2004.

J. Morel and J. Warsa, "An Sn Spatial Discretization Scheme for Tetrahedral Meshes," to appear in *Nuclear Science and Engineering*.

J. Morel and J. Warsa, "Sn Finite-Element Lumping on Quadrilateral Meshes in \$X-Y\$ Geometry," accepted for presentation, MC2005: International Topical Meeting on Mathematics and Computation, Supercomputing, Reactor Physics, and Nuclear and Biological Applications, Avignon, France, September 12-15, 2005.

B. Nadiga, D. Livescu, and C. McKay, "Stochastic Large Eddy Simulations of Geostrophic Turbulence," to be presented at the 2005 General Assembly meeting of the European Geophysical Union, Vienna, Austria, April 2005.

B. Nadiga, D. Livescu, and C. McKay, "Stochastic Large Eddy Simulations of Geostrophic Turbulence," to be presented at the 2005 Joint Assembly meeting of the American Geophysical Union, New Orleans, May 2005.

J. Ristorcelli and D. Livescu, "Decay of Isotropic Turbulence: A Tale of Two Decays," Cascade Dynamics: Fundamentals and Modeling Workshop, Santa Fe, N.M., August 16-19, 2004.

J. Ristorcelli and D. Livescu, "Decay of Isotropic Turbulence: Fixed Points and Solutions for Non-Constant G_R Palinstrophy," *Physics of Fluids*, 16(9), 3487-3490, 2004.

J. Ristorcelli and D. Livescu, "Decay of Isotropic Turbulence: Fixed Points and Solutions for Non-Constant Palinstrophy," *Bulletin of American Physical Society*, 49(10), 112, 2004. (Also presented at the 57th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Seattle, Wash., November 21-23, 2004.)

M. Rosa, Y. Azmy, and J. Morel, "Properties of the Sn-Equivalent Integral Transport Operator in Heterogeneous Slabs," accepted for presentation, MC2005:International Topical Meeting on Mathematics and Computation, Supercomputing, Reactor Physics, and Nuclear and Biological Applications, Avignon, France, September 12-15, 2005.

M. Rosa, Y. Azmy, and J. Morel, "Properties of the Sn-Equivalent Integral Transport Operator in Slab Geometry," accepted for presentation at the American Nuclear Society Annual Meeting, San Diego, Calif., June 5-9, 2005.

R. Rubinstein, T. Clark, D. Livescu, and L. Luo, "Time-Dependent Isotropic Turbulence," *Journal of Turbulence* 5, 011, 1-16, 2004.

R. Ward, R. Baker, and J. Morel, "A Diffusion Synthetic Acceleration Method for Block Adaptive Mesh Refinement," submitted to *Nuclear Science and Engineering*.

J. Warsa, M. Benzi, T. Wareing, and J. Morel, "Preconditioning a Mixed Discontinuous Finite Element Method for Radiation Diffusion," to appear in *Journal on Numerical Linear Algebra with Applications*.

J. Warsa, T. Wareing, and J. Morel, "Krylov Iterative Methods and the Degraded Effectiveness of Diffusion Synthetic Acceleration for Multidimensional Sn Calculations in Problems with Material Discontinuities," *Nuclear Science and Engineering*, 147, 218-248, 2004.

J. Warsa, T. Wareing, J. Morel, J. McGhee, and R. Lehoucq, "Krylov Subspace Iterations for Deterministic k-Eigenvalue Calculations," *Nuclear Science and Engineering*, 147, 26-42 (2004).

Climate and Ocean Modeling Team

S. Belviso, S. Elliott, et al, "Comparison of Global Climatological Maps of Sea Surface Dimethylsulfide," *Global Biogeochemical Cycles*, 18: 10.1029/2003GB002193.

R. Bleck, M. Maltrud, S. Chu, F. Chai, F. Chavez, and S. Elliott, "Comparison of Cartesian and Isopycnal Simulations of Oceanic Carbon Sequestration via Iron Fertilization and Deep Injection," University of Miami web page.

C. Cao, D. Holm, and E. Titi, "Traveling Wave Solutions for a Class of One-Dimensional Nonlinear Shallow Water Wave Models," *J. of Dyn. and Diff. Eqns.*, 16, 167-178, 2004.

S. Chu, S. Elliott, M. Maltrud, and F. Chai, "Iron Patch Enrichments in the Southern Ocean of a Global Eddy Permitting General Circulation Model," in *ESEC*, Vol. 2, FiatLux: Chapter 8.

S. Chu, S. Elliott, M. Maltrud, and D. Erickson, "Ecodynamic and Eddy Admitting Simulations of Dimethyl Sulfide Distributions in the Parallel Ocean Program," *Earth Interactions*, 8: 1-25.

R. Cushman, H. Dullin, A. Giacobbe, D. Holm, M. Joyeux, P. Lynch, D. Sadovskii, and B. Zhilinskii, "The CO₂ Molecule as a Quantum Realization of the 1:1:2 Resonant Swing-Spring with Monodromy," *Phys. Rev. Lett.* 93, 024302-5, 2004. (This four-page paper received a two-page review in Ian Stewart, *Nature* 430, 731-732, 2004.)

H. Dullin, G. Gottwald, and D. Holm, "On Asymptotically Equivalent Shallow Water Wave Equations," *Physica D* 190, 1-14, 2004.

S. Elliott and S. Chu, "Algorithms for Analytical Optimization of Large Scale Marine Trace Gas Cycling Constants," technical report, LA-UR-05-2044, Los Alamos National Laboratory.

S. Elliott, S. Chu, and D. Erickson, "Contours of Simulated Marine Dimethyl Sulfide Distributions under Variation in a Gabric Mechanism," technical report, technical report, LA-UR-05-1582, Los Alamos National Laboratory.

S. Elliott, S. Chu, M. Maltrud, and A. McPherson, "Animation of Global Marine Chlorophyll Distributions from Fine Grid Biogeochemistry/Transport Modeling," in *ESEC*, Vol. 2, FiatLux: Chapter 9.

S. Elliott, M. Maltrud, S. Chu, and D. Erickson, "A Marine Trace Gas Cycling Module for Community Climate System Simulations," technical report, LA-UR-04-8200, Los Alamos National Laboratory.

S. Elliott, M. Maltrud, S. Chu, and D. Erickson, "TRACEGAS_MOD: Processing for Low Concentration Volatiles in the Community Climate System Model Ocean," submitted to *Environmental Modeling and Software*. (Also a technical report, LA-UR-05-0673, Los Alamos National Laboratory.)

P. Gent, F. Bryan, G. Danabasoglu, K. Lindsay, D. Tsumune, M. Hecht, S. Doney, "Ocean Chlorofluorocarbon and Heat Uptake During the 20th Century in the CCSM3," submitted to the *Journal of Climate*. (Also a technical report, LA-UR-05-0888, Los Alamos National Laboratory.)

B. Geurts and D. Holm, "Nonlinear Regularization for Large-Eddy Simulation in Direct and Large-Eddy Simulation V," in Proceedings of DLES5, Munich, August 27-29, 2003, R. Friedrich, B. J. Geurts, and O. Metais (editors), Kluwer Academic Publishers, pp 5-14, 2004.

M. Hecht, review (written at the request of the American Meteorological Society) of S. Griffies' book, "Fundamentals of Ocean Climate Models," Princeton University Press. Review to appear in the *Bulletin of the American Meteorological Society*.

D. Holm, "The Euler-Poincare Variational Framework for Modeling Fluid Dynamics," in Geometric Mechanics and Symmetry: The Peyresq Lectures, J. Montaldi and T. Ratiu (editors), London Mathematical Society Lecture Notes Series 306, Cambridge University Press, 2005.

D. Holm, "Taylor's Hypothesis, Hamilton's Principle, and the LANS-Alpha Model for Computing Turbulence," Science-Based Prediction for Complex Systems, N. Cooper (editor), *Los Alamos Science* 29, 172-180, 2005.

D. Holm and B. Fabijonas, " Craik-Criminale Solutions and Elliptic Instability in Nonlinear-Reactive Closure Models for Turbulence," *Phys. Fluids* 16, 853-866, 2004.

D. Holm and B. Fabijonas, "Euler-Poincare Formulation and Elliptic Instability for Nth-Gradient Fluids," *J. Phys. A: Math. Gen.* 37, 7609-7623, 2004.

D. Holm and B. Fabijonas, "Multi-Frequency Craik-Criminale Solutions of the Navier-Stokes Equations," *J. Fluid Mech.* 506, 207-215, 2004.

D. Holm and A. Hone, "A Class of Equations with Peakon and Pulson Solutions," (with an appendix by H. Braden and J. Byatt-Smith, *D. D. J. of Nonlin. Math. Phys.* 12, Supplement 1, 1-15, 2005.

D. Holm, C. Jeffery, S. Kurien, D. Livescu, M. Taylor, and B. Wingate, "The LANS-Alpha Model for Computing Turbulence—Origins, Results, and Open Problems," Science-Based Prediction for Complex Systems, N. Cooper (editor), *Los Alamos Science* 29, 152-171, 2005.

D. Holm and J. Marsden, "Momentum Maps and Measure Valued Solutions (Peakons, Filaments, and Sheets) of the Euler-Poincare Equations for the Diffeomorphism Group," in *The Breadth of Symplectic and Poisson Geometry*, a Festschrift, for A. Weinstein, J. Marsden, and T. Ratiu (editors), Birkhauser Boston, *Progr. Math.* 232, 203-235, 2004.

D. Holm, V. Putkaradze, and S. Stechmann, "Rotating Concentric Circular Peakons," *Nonlinearity* 17, 1-24, 2004.

D. Holm, J. Rananather, A. Troune, and L. Younes, "Soliton Dynamics in Computational Anatomy," *NeuroImage* 23, S170-178, 2004.

D. Holm and B. Wingate, "Baroclinic Instabilities of the Two-Layer Quasigeostrophic Alpha Model," to appear in the *Journal of Physical Oceanography*, 2005.

B. Nadiga, "Proposal for Organizing 'Stochastic Closure for Large Scale Turbulent Flows,'" accepted for AGU Joint Assembly, New Orleans, 2005.

B. Nadiga, "Proposal for Organizing 'Stochastic Dynamics,'" accepted for EGU, Vienna, Austria, 2005.

B. Nadiga and D. Straub, "Organized 'Dynamics of Ocean Circulation,'" AGU Joint Assembly, Montreal, Canada, May 2004.

M. Petersen, K. Julien, and J. Weiss, "Vortex Cores, Strain Cells, and Filaments in Quasi-Geostrophic Turbulence," submitted to *Physics of Fluids*.

M. Petersen, B. Kraus, and T. Windham, "Striving Towards Equity; Underrepresented Minorities and Mathematics," SIAM News, March (Part I), April (Part II).

M. Taylor, B. Wingate, L. Bos, "A New Algorithm for Computing Multivariate Quadrature Points," submitted to the *SIAM Journal on Numerical Analysis*, 2004.

B. Wingate, "The Maximum Allowable Time Step for the Shallow Water Alpha-Model and Its Relation to Time-Implicit Differencing," *Monthly Weather Review*, Vol. 132, pp. 2719, 2004.

Hydro Methods for Thermonuclear Applications Team

M. Christie, J. Glimm, J. Grove, D. Higdon, D. Sharp, and M. Wood-Schultz, "Error Analysis and Simulations of Complex Phenomena," *Los Alamos Science*, 29:2-25, 2005.

E. Dendy, "Interface Models and Hydrodynamic Coupling for the Crestone Project (U)," limited-distribution report, LA-CP-05-0308, Los Alamos National Laboratory.

E. Dendy, "The RAGE Hydrodynamics Algorithm," a technical report, LA-UR-05-1642, Los Alamos National Laboratory.

S. Dutta, E. George, J. Glimm, J. Grove, H. Jin, T. Lee, X. Li, D. Sharp, K. Ye, Y. Yu, Y. Zhang, and M. Zhao, "Shock Wave Interactions in Spherical and Perturbed Spherical Geometries," *Nonlinear Analysis*, 2004. (In press: University at Stony Brook preprint number SB-AMS-04-09. Also, a technical report, LA-UR-04-2989, Los Alamos National Laboratory.)

S. Dutta, J. Glimm, J. Grove, D. Sharp, and Y. Zhang, "Error Comparison in Tracked and Untracked Spherical Simulations," *Computers and Mathematics with Applications*, 48:1733-1747, 2004. (University at Stony Brook preprint number AMS-03-10. Also, a technical report, LA-UR-03-2920, Los Alamos National Laboratory.)

S. Dutta, J. Glimm, J. Grove, D. Sharp, and Y. Zhang, "Spherical Richtmyer-Meshkov Instability for Axisymmetric Flow," *Mathematics and Computers in Simulations*, 65:417-430, 2004. (University at Stony Brook preprint number AMS-03-13.)

J. Glimm, J. Grove, Y. Kang, T. Lee, X. Li, D. Sharp, Y. Yu, K. Ye, and M. Zhao, "Errors in Numerical Solutions of Spherically Symmetric Shock Physics Problems," *Contemporary Mathematics*, 371:163-179, 2005. (University at Stony Brook preprint number SB-AMS-04-03. Also, a technical report, LA-UR-04-0713, Los Alamos National Laboratory.)

J. Glimm, J. Grove, Y. Kang, T. Lee, X. Li, D. Sharp, Y. Yu, K. Ye, and M. Zhao, "Statistical Riemann Problems and a Composition Law for Errors in Numerical Solutions of Shock Physics Problems," *SISC*, 26:666-697, 2004. (University at Stony Brook preprint number SB-AMS-03-11. Also, a technical report, LA-UR-03-2921, Los Alamos National Laboratory.)

X. Li, J. Wohlbier, S. Jin, and J. Booske, "Eulerian Method for Computing Multi-valued Solutions of the Euler-Poisson Equations and Applications to Wave Breaking in Klystrons," *Phys. Rev. E* 70, 016502, 2004.

A. Singh, J. Scharer, J. Booske, and J. Wohlbier, "Second and Third-Order Signal Injection for Nonlinear Distortion Suppression in a Traveling Wave Tube," *IEEE Trans. Electron Devices*, Vol. 52, No. 5, 2005.

A. Singh, J. Wohlbier, J. Booske, and J. Scharer, "Experimental Verification of the Mechanisms for Nonlinear Harmonic Growth and Suppression by Harmonic Injection in a Traveling Wave Tube," *Phys. Rev. Lett.* 92, 205005, 2004.

J. Wohlbier and J.H. Booske, "Mechanisms for Phase Distortion in a Traveling Wave Tube," *Phys. Rev. E* 69, 066502, 2004.

J. Wohlbier and J. Booske, "Nonlinear Space Charge Wave Theory of Distortion in a Klystron," *IEEE Trans. Electron Devices*, Vol. 52, No. 5, 2005.

J. Wohlbier, J. Booske, and I. Dobson, "On the Physics of Harmonic Injection in a Traveling Wave Tube," *IEEE Trans. Plasma Sci.*, 32(3):1073-1085, 2004.

J. Wohlbier, S. Jin, and S. Sengele, "Eulerian Calculations of Wave Breaking and Multi-valued Solutions in a Traveling Wave Tube," *Physics of Plasmas* 12, 023106, 2005.

Y. Zhang, P. Drake, J. Glimm, J. Grove, and D. Sharp, "Radiation Coupled Front Tracking Simulations for Laser Driven Shock Experiments," in press, *J. Nonlinear Analysis*, 2005. (Also, a technical report, LA-UR-04-2381, Los Alamos National Laboratory.)

Data-Driven Modeling Team

LANL Reports

K. Borozdin, et al., "Information Extraction from Muon Radiography Data," technical report, LA-UR-04-3985. Los Alamos National Laboratory.

T. Asaki, "Clustering and Likelihood Based Analysis for Muon Radiography," technical report, LA-UR-05-2659, Los Alamos National Laboratory.

T. Asaki, "Elasticity Based TSWarp Cost Functions," technical report, LA-UR-04-4099, Los Alamos National Laboratory.

T. Asaki, "The Geometry of a Beta-Layered Solid Grown on a Perturbed Boundary," technical report, LA-UR-04-4101, Los Alamos National Laboratory.

T. Asaki, "Inverse Abel Transform Regularization," technical report, LA-UR-04-4100, Los Alamos National Laboratory.

T. Asaki and K. Vixie, "SVD Analysis for Radiographic Object Reconstruction III: Total Variation Regularization," technical report, LA-UR-04-7076, Los Alamos National Laboratory.

K. Vixie and T. Asaki, "Defensible Metrics and Merit Functions: Making Informative Comparisons of Computer Simulations and Experiments," technical report, LA-UR-04-8498, Los Alamos National Laboratory. (Also, an LDRD Progress Report in LA-05-0001-PR.)

Journal Papers

T. Asaki, P. Campbell, R. Chartrand, C. Powell, K. Vixie, and B. Wohlberg, "Abel Inversion Using Total Variation Regularization: Applications," submitted to *Inverse Problems in Science and Engineering*. (Also, a technical report, LA-UR-05-2657, Los Alamos National Laboratory.)

T. Asaki, R. Chartrand, C. Powell, K. Vixie, and B. Wohlberg, "Abel Inversion Using Total Variation Regularization," submitted to *Inverse Problems in Science and Engineering*. (Also, a technical report, LA-UR-05-0680, Los Alamos National Laboratory.)

Talks and Presentations

T. Asaki and R. Chartrand, "Tomographic Methods for Limited View Angles and Sparse Data," Montana State University, invited talk, September 2004. (Also, a technical paper, LA-UR-04-5767, Los Alamos National Laboratory.)

Borozdin, et al., "Information Extraction from Muon Radiography Data," Int. Conf. on Cybernetics and Inf. Tech., Systems and Applications, Orlando, Fla., July 2004.

R. Chartrand and T. Asaki, "Background Radiography for Border Inspections," Montana State University, invited talk, September 2004. (Also, a technical report, LA-UR-04-5766, Los Alamos National Laboratory.)

R. Chartrand, et al., "Detecting Nuclear Materials from Muon-Scattering Data," AAAS annual meeting, Washington, D.C., February 2005.

Hogan, et al., "Detecting Special Nuclear Materials by Muon Radiography," APS Meeting, Denver, May 2004. (Also a technical report, LA-UR-04-2975, Los Alamos National Laboratory.)

Schirato, et al., "Development of Cosmic Ray Muon Radiography for the Detection of High-Z Objects," Ninth Topical Seminar on Innovative Particle and Radiation Detectors, Siena, Italy, May 2004.

Schultz, et al., "Cosmic Ray Muon Radiography for the Detection of Contraband SNM," INEEL/IAC/DTRA 2004 Active Interrogation Workshop, Idaho Falls, Idaho, June 2004.

Schultz, et al. "Cosmic Ray Muon Radiography: Image Reconstruction and Material Discrimination," SIAM Conference on Imaging Science, Salt Lake City, Utah, May 2004.

Schultz, et al., "Detection of Dense, High-Z Objects with Muon Radiography," Los Alamos National Laboratory Workshop on Active Techniques for Diagnostics and Detection of Special Nuclear Materials and Explosives, Los Alamos, N.M., May 2004.

Schultz, et al., "Image Reconstruction and Material Z Discrimination via Cosmic Ray Muon Radiography," *Nuclear Instruments and Methods A* 519:3, 687, March 2004. (Also, a technical report, LA-UR-03-4806, Los Alamos National Laboratory.)

Modeling, Algorithms, and Informatics (CCS-3)

Refereed/Peer Journals

F. Alexander, G. Eyink, and J. Restrepo, "Accelerated Monte-Carlo for Optimal Estimation of Time Series," *Journal of Statistical Physics*, 2004, to appear.

F. Alexander, A. Garcia, and D. Tartakovsky, "Algorithm Refinement for Stochastic Partial Differential Equations: II Correlated Systems," *Journal of Computational Physics*, 2004, to appear.

F. Alexander, A. Garcia, and D. Tartakovsky, "Noise in Algorithm Refinement Methods," *Computing in Science and Engineering*, to appear 2005.

M. Anghel, Y. Ben-Zion, and R. Rico-Martinez, "Dimensional Reduction, Nonlinear System Identification and Forecasting of Earthquake Fault Dynamics," *Pure and Applied Geophysics*, 161, 2023-2051, 2004.

L. Arber and S. Pakin, "The Impact of Message-Buffer Alignment on Communication Performance," *Parallel Processing Letters*, to appear in June 2005. (Also a technical report, LA-UR-04-6066, Los Alamos National Laboratory.) Available from <http://www.c3.lanl.gov/~pakin/papers/ppl2005.pdf>.

J. Beecroft, D. Addison, D. Hewson, M. McLaren, F. Petrini, and D. Roweth, "Quadrics QsNet II: Pushing the Limit of the Design of High-Performance Networks for Supercomputers," *IEEE Micro*, to appear in 2005.

A. Christmann and I. Steinwart, "On Robustness Properties of Convex Risk Minimization Methods for Pattern Recognition," *Journal of Machine Learning Research*, 5:1007-1034, 2004.

G. Eyink, J. Restrepo, and F. Alexander, "A Mean-Field Approximation in Data Assimilation for Nonlinear Dynamics," *Physica D*, to appear.

G. Eyink, J. Restrepo, and F. Alexander, "A Statistical-Mechanical Approach to Data Assimilation for Nonlinear Dynamics: II. Evolution Approximations," submitted to the *Journal of Statistical Physics*, 2004.

S. Ferson, C. Joslyn, J. Helton, W. Oberkamp, and K. Sentz, "Summary of the Epistemic Uncertainty Workshop: Consensus Amid Diversity," *Reliability Engineering and Systems Safety*, Vol. 85:1-3, pp. 355-370, 2004.

E. Frachtenberg, D. Feitelson, F. Petrini, and J. Fernandez, "Adaptive Parallel Job Scheduling with Flexible Co-Scheduling," in *IEEE Transactions on Parallel and Distributed Systems*, to appear 2005.

L. Guo, S. Jiang, L. Xiao, and X. Zhang, "Fast and Low Cost P2P Searching by Exploiting Localities in Peer Community and Individual Peers," *Journal of Parallel and Distributed Computing*, to appear 2005.

M. Guo, L. Yang, M. Buecker, J. Cao, W. Chang, V. Chaudhary, B. Di Martino, W. Jia, D. Kerbyson, J. Li, T. Rauber, and G. Runga (editors), "Hardware/Software Support for High Performance Scientific and Engineering Computing," *IEICE Transactions on Information Systems*, Vol. 87, July 2004.

L. Gurvits, "Classical Complexity and Quantum Entanglement," *Journal of Computer and System Sciences*, 2004.

L. Gurvits, "Combinatorial and Algorithmic Aspects of Hyperbolic Polynomials," *Electronic Colloquium on Computational Complexity*, Volume 11, 2004.

L. Gurvits, "The Van der Waerden Conjecture for Mixed Discriminants," *Advances in Mathematics*, in press, 2005.

L. Gurvits and J. Ledoux, "Markov Property for a Function of a Markov Chain: A Linear Algebra Approach," *Linear Algebra and its Applications*, in press, 2005.

L. Gurvits and L. Rodman, "On Matrix Polynomials with Real Roots," *SIAM Journal of Matrix Analysis*, Vol. 26, No. 3, pp. 758-764, 2005.

D. Hush and C. Scovel, "Fat-Shattering of Affine Functions," *Combinatorics Probability and Computing*, Vol. 13, pp. 353-360, 2004.

S. Jiang and X. Zhang, "Making LRU Friendly to Weak Locality Workloads: A Novel Replacement Algorithm to Improve File Buffer Cache Performance," *IEEE Transactions on Computers*, to appear 2005.

S. Jiang and X. Zhang, "Token-Ordered LRU: An Efficient Page Replacement Policy and Implementation in Linux Systems," in *Performance Evaluation*, 60 (1-4): 5-29. To appear May 2005.

C. Joslyn, S. Mniszewski, A. Fulmer, and G. Heaton, "The Gene Ontology Categorizer," *Bioinformatics*, Vol. 20:s1, pp. 169-177, 2004.

D. Kerbyson, A. Hoisie, S. Pakin, F. Petrini, and H. Wasserman, "A Performance Evaluation of an Alpha EV7 Processing Node," the *International Journal of High Performance Computing Applications*, 18(2):199-209, May 1, 2004. (Available from http://www.c3.lanl.gov/~pakin/papers/ijhpca_ev7.pdf.)

D. Martin, P. Colella, M. Anghel, and F. Alexander, "Adaptive Mesh Refinement for Multiscale Nonequilibrium Physics," *Computers in Science and Engineering*, in press. (Also a technical report, LA-UR-05-0749, Los Alamos National Laboratory.)

D. Martin, P. Colella, M. Anghel, and F. Alexander, "Adaptive Mesh Refinement for Multiscale Nonequilibrium Physics," *Computing in Science and Engineering*, to appear in 2005.

W. Oberkampf, J. Helton, C. Joslyn, S. Wojtkiewicz, and S. Ferson, "Uncertainty in System Response Given Uncertain Parameters," *Reliability Engineering and System Safety*, Vol. 85:1-3, pp.~11-20, 2004.

M. Pernice and R. Hornung, "Newton-Krylov-FAC Methods for Problems Discretized on Locally Refined Grids," *Computing and Visualization in Science*, to appear in 2005.

F. Petrini, J. Fernandez, A. Moody, E. Frachtenberg, and D. Panda, "NIC-based Reduction Algorithms for Large-Scale Clusters," *International Journal of High Performance Computing and Networking*, to appear 2005.

I. Steinwart, D. Hush, and C. Scovel, "A Classification Framework for Anomaly Detection," *Journal of Machine Learning Research*, 6:211-232, 2005.

I. Steinwart, "Consistency of Support Vector Machines and other Regularized Kernel Machines," *IEEE Transactions on Information Theory*, 51:128-142, 2005.

I. Steinwart, "Entropy of Convex Hulls—Some Lorentz Norm Results," *Journal of Approximation Theory*, 128:42-52, 2004.

K. Summers, T. Caudell, K. Berkbigger, B. Bush, K. Davis, and S. Smith, "Graph Visualization for the Analysis of the Structure and Dynamics of Extreme-Scale Supercomputers," *Information Visualization*, 3, pp. 209-222, 2004.

B. Uberuaga, M. Anghel, and A. Voter, "Synchronization of Trajectories in Canonical Molecular Dynamics Simulations," *Journal of Chemical Physics*, 120, 6363, 2004.

K. Verspoor, "Toward a Semantic Lexicon for Biological Language Processing," *Comparative and Functional Genomics*, Vol. 6, issue 1-2, pp. 61-66. DOI: 10.1002/cfg.451.

K. Verspoor, J. Cohn, C. Joslyn, S. Mniszewski, A. Rechtsteiner, L. Rocha, and T. Simas, "Protein Annotation as Term Categorization in the Gene Ontology Using Word Proximity Networks," *BMC Bioinformatics*, to appear in 2005.

T. Warnock, R. Nemzek, J. Dreicer, and D. Torney, "Distributed Sensor Networks for Detection of Mobile Radioactive Sources," *IEEE Transactions on Nuclear Science*, 51, pp. 1693-1700, August 2004.

C. Winter, E. Springer, K. Costigan, P. Fasel, S. Mniszewski, and G. Zyvoloski, "Virtual Watersheds: Simulating the Water Balance of the Rio Grande Basin," *IEEE Computers in Science and Engineering*, Vol. 6, Number 3, pp. 18-26, May/June 2004.

Technical Reports

K. Atkins, C. Barrett, J. Cohn, C. Homan, S. Kothapally, A. Marathe, M. Marathe., S. Mniszewski, and P. Romero, Marketecture Version 2.0, June 2004.

K. Atkins, J. Cohn, C. Homan, S. Kothapally, A. Marathe, and S. Mniszewski, Urban Infrastructure Suite: Financial/Energy Sector, Marketecture: Chicago Case Study, May 2004.

K. Berkbigher, et. al., Urban Population Mobility Simulation Technologies Volume 4: Population Generation, technical documentation, also in LA-UR-04-6039, Los Alamos National Laboratory.

M. Cannon and T. Warnock, "A Shape Descriptor Based on the Line Scan Transform," a technical report, LA-UR-04-5865, Los Alamos National Laboratory.

M. Cannon, T. Warnock, and S. Kumar, "A New Shape Metric Based on the Line Scan Transform (U)," technical report, LA-UR-04-3931, Los Alamos National Laboratory.

A. Christmann and I. Steinwart, "Consistency and Robustness of Kernel Based Regression," a technical report, LA-UR 04-8797, Los Alamos National Laboratory. Submitted to *Annals of Statistics*.

K. Davis, A. Hoisie, G. Johnson, D. Kerbyson, M. Lang, S. Pakin, and F. Petrini, "Lightning: A Performance and Scalability Report on the Use of 1020 Nodes," technical report, LA-UR-04-1652, Los Alamos National Laboratory.

K. Davis, A. Hoisie, G. Johnson, D. Kerbyson, M. Lang, S. Pakin, and F. Petrini, "Lightning: Performance Results for the Level 2 Milepost," technical report, LA-UR-04-5064, Los Alamos National Laboratory.

E. Frachtenberg. "Process Coordination for Commodity Systems," a technical report, LA-UR-04-7256, Los Alamos National Laboratory, December 2004.

A. Hoisie and S. Pakin, "Performance Modeling of a 2010-era ASC Supercomputer (U)," internal report, LA-CP-05-0172, Los Alamos National Laboratory.

G. Johnson, M. Lang, and D. Kerbyson, "Empirical Analysis of Various Memory Models on an Intel EM64T Based Processing Node," technical report, LA-UR-04-7449, Los Alamos National Laboratory.

C. Joslyn, "A Formerly Breathless Introduction to Generalized Information Theory," technical report, LA-UR-04-4078, Los Alamos National Laboratory, <ftp://ftp.c3.lanl.gov/pub/users/joslyn/shortcourse.pdf>.

C. Joslyn, "GIT Analysis of the Crushable Foam Experiment and Simulations," technical report, LA-UR-04-6207, Los Alamos National Laboratory, <ftp://ftp.c3.lanl.gov/pub/users/joslyn/foam.pdf>.

C. Joslyn, J. Oliverira, and C. Scherrer, "Order Theoretical Knowledge Discovery: A White Paper," technical report, LA-UR-04-5812, Los Alamos National Laboratory, <ftp://ftp.c3.lanl.gov/pub/users/joslyn/white.pdf>.

C. Joslyn, K. Verspoor, S. Mniszewski, and J. Cohn, "Automated Protein Function Annotation via Markov Adjusted Ontology Categorization," a technical report, LA-UR-05-0639, Los Alamos National Laboratory.

D. Kerbyson, "A Note on the Different Task Mappings of SAGE onto BG/L," technical report, LA-UR-04-4118, Los Alamos National Laboratory.

D. Kerbyson, "An Initial Analysis of Application Communication Degree," technical report, LA-UR-04-7456, Los Alamos National Laboratory.

D. Kerbyson, "Discussion Document 1: Modeling the PERCS Networks," internal report, LA-CP-04-0941, Los Alamos National Laboratory.

D. Kerbyson and K. Barker, "Automatic Identification of Application Communication Patterns via Templates," technical report, LA-UR-04-7451, Los Alamos National Laboratory.

D. Kerbyson and A. Hoisie, "An Initial Analysis of the BG/P System," technical report, LA-UR-04-5140, Los Alamos National Laboratory.

D. Kerbyson, M. Lang, G. Johnson, "A Note on the Performance of the EM64T (Nacona) Node," technical report, LA-UR-04-7450, Los Alamos National Laboratory.

D. Kerbyson and P. Jones, "An Initial Performance Model of POP," technical report, LA-UR-04-4119, Los Alamos National Laboratory.

D. Kerbyson and P. Jones, "A Performance Model of the Parallel Ocean Program," technical report, LA-UR-04-8793, Los Alamos National Laboratory.

D. Kerbyson and M. Lang, "An Initial Performance Analysis of Commodity Memories in Intel Processing Nodes," technical report, LA-UR-04-2111, Los Alamos National Laboratory.

M. Mathis and D. Kerbyson, "A General Performance Model of Structured and Unstructured Mesh Particle Transport Computations," technical report, LA-UR-04-8794, Los Alamos National Laboratory.

S. Mniszewski, "POset Ontology Categorizer (POSOC) Software Design Notes," included with the POSOC Open Source Distribution, technical report, LA-UR-04-8799, Los Alamos National Laboratory.

M. Pernice and B. Philip, "Solution of Equilibrium Radiation Diffusion Problems Using Implicit Adaptive Mesh Refinement," technical report, LA-UR-04-3620, Los Alamos National Laboratory.

C. Scovel, D. Hush, and I. Steinwart, "Learning Rates for Density Level Detection," a technical report, submitted for publication as a technical report (an LA-UR in 2005), at Los Alamos National Laboratory.

D. Spooner and D. Kerbyson, "Performance Feature Identification by Comparative Analysis," technical report, LA-UR-04-7522, Los Alamos National Laboratory.

I. Steinwart, D. Hush, and C. Scovel, "An Explicit Description of the Reproducing Kernel Hilbert Spaces of Gaussian RBF Kernels," a technical report, LA-UR 04-8274, Los Alamos National Laboratory. Submitted to *IEEE Transactions on Information Theory*.

I. Steinwart and C. Scovel, "Fast Rates for Support Vector Machines," a technical report, LA-UR 05-0451, Los Alamos National Laboratory. Submitted to the Conference on Learning Theory.)

I. Steinwart and C. Scovel, "Fast Rates for Support Vector Machines Using Gaussian Kernels," a technical report, LA-UR 04-8796, Los Alamos National Laboratory. Submitted to *Annals of Statistics*.

K. Verspoor, C. Joslyn, J. Ambrosiano, A. Backer, O. Bodenreider, L. Hirschman, P. Karp, H. Kelly, S. Loranger, M. Musen, R. Sriram, and C. Wroe, "Knowledge Integration for Biothreat Response," technical report, LA-UR-05-0907, Los Alamos National Laboratory.

Book Chapters/Edited Books/Book Reviews

A. Christmann and I. Steinwart, "Support Vector Machines: Theory and Applications," a book in preparation for Springer, New York, N.Y.

J. Fernandez, F. Petrini, E. Frachtenberg, "Achieving Predictable and Scalable Performance with BCS-MPI," in *Engineering the Grid: Status and Perspective*, B. Di Martino, J. Dongarra, A. Hoisie, L. Yang, H. Zima (editors), to appear 2005.

C. Joslyn, "Poset Ontologies and Concept Lattices as Semantic Hierarchies," in *Conceptual Structures at Work, Lecture Notes in Artificial Intelligence*, Vol. 3127, Wolff, Pfeiffer, and Delugach (editors), pp. ~287-302, Springer-Verlag, Berlin.

C. Joslyn and J. Booker, "Generalized Information Theory for Engineering Modeling and Simulation," in *Engineering Design Reliability Handbook*, E. Nikolaidis et al. (editors), pp. 9:1-40, CRC Press.

C. Joslyn and W. Bruno, "Weighted Pseudo-Distances for Categorization in Semantic Hierarchies," to appear in 2005 International Conference on Conceptual Structures, *Lecture Notes in Artificial Intelligence*.

Conference Proceedings, Talks, Etc.

M. Anghel, "A Bayesian Contribution to Performance Modeling," invited talk given at the Fifth Symposium of the Los Alamos Computer Science Institute: LACSI 2004, October 12-14, Santa Fe, N.M. (Also, a technical report, LA-UR-04-7199, Los Alamos National Laboratory.)

M. Anghel, S. Mniszewski, D. Kerbyson, and F. Alexander, "A Bayesian Contribution to Performance Analysis," Los Alamos Computer Science Institute Symposium (LACSI 2004), Workshop on Performance and Productivity of Extreme-Scale Parallel Systems, October 2004.

S. Boettcher, G. Istrate, and A.G. Percus, "Spines of Random Constraint Satisfaction Problems: Definition and Impact on Computational Complexity," in *Proceedings of the Eighth International Symposium on Artificial Intelligence and Mathematics (AIMATH '04)*, AI&M 2-2004. Also to appear in 2005 in *Annals of Mathematics and Artificial Intelligence*.

S. Boettcher and A. Percus, "Extremal Optimization at the Phase Transition of the 3-Coloring Problem," *Physical Review E* 69, 066703, 2004.

A.

Cannon and D. Hush, "Multiple-Instance Learning with Simple Classifiers," submitted and accepted for publication in ICMLA-2004 (for the 2004 International Conference on Machine Learning Applications).

J. Cohn, C. Joslyn, S. Mniszewski, and K. Verspoor, "Making the CASP Functional Annotation Process into a Widget," PFIG meeting, February 2005.

J. Cohn, C. Joslyn, S. Mniszewski, and K. Verspoor, "Predicting Protein Function Using Nearest Neighbor Categorization," poster at Bioscience Division Review, March 2005.

J. Cohn, K. Verspoor, S. Mniszewski, and C. Joslyn, "Predicting Protein Function Using Nearest Neighbor Categorization," poster at Second Annual Rocky Mountain Regional Bioinformatics Conference, December 2004.

K. Davis, A. Hoisie, G. Johnson, D. Kerbyson, M. Lang, S. Pakin, and F. Petrini, "A Performance and Scalability Analysis of the BlueGene/L Architecture," in Proceedings of SuperComputing (SC2004), Pittsburgh, Pa., November 6-12, 2004. (Also, a technical report, LA-UR-04-5620, Los Alamos National Laboratory.) Available at: <http://www.sc-conference.org/sc2004/schedule/pdfs/pap302.pdf>.

K. Davis and F. Petrini, "Achieving Usability and Efficiency in Large-Scale Parallel Computing Systems (Tutorial)," Europar 2004, Pisa, Italy.

K. Eggert, E. Beighley, T. Dunne, L. Mertes, K. Verdin, K., and S. Mniszewski, "Application of a Continental Scale River Modeling Framework to the Purus River Basin—A Major Tributary of the Amazon River," NCAR CCSM Land Working Group Meeting, March 2005.

K. Eggert, E. Beighley, T. Dunne, K. Verdin, and S. Mniszewski, "A Continental Scale River Modeling Framework Designed around Topographic Modeling Units with Both Hydrologic and Hydraulic Realism," NCAR Ninth Annual CCSM Workshop, July 2004.

E. Frachtenberg. "Designing Parallel Operating Systems Using Modern Interconnects," in Computer Science and Artificial Intelligence Laboratory (CSAIL), Massachusetts Institute of Technology, Cambridge, Mass., September 2004.

E. Frachtenberg. "Toward Realistic Evaluation of Job Scheduling Strategies," in a seminar talk, given at the Computer Science Departments of Hebrew University (Jerusalem), Tel Aviv University (Tel Aviv), Technion, Israel Institute of Technology (Haifa), Interdisciplinary Center (Herzlia), and Ben Gurion University, (Beer Sheva), Israel, December 2004.

E. Frachtenberg. "Using Multi-Rail Networks in High-Performance Clusters," in ClubNet, Department of Electrical Engineering, Technion Israel Institute of Technology, Haifa, Israel, December 2004.

R. Gioiosa, F. Petrini, K. Davis, and F. Lebaillif-Delamare, "Analysis of System Overhead on Parallel Computers," in the Fourth IEEE International Symposium on

Signal Processing and Information Technology (ISSPIT 2004), Rome, Italy, December 2004.

N. Gulbahce, F. Alexander, G. Johnson, "A Space-Time Cluster Monte Carlo Algorithm for Optimal Estimation," in preparation.

N. Gulbahce, W. Klein, and H. Gould, "Heterogeneity in Classical and Non-Classical Nucleation," cond-mat/0407304.

L. Guo, S. Jiang, L. Xiao, and X. Zhang, "Exploiting Content Localities for Efficient Search in P2P Systems," in Proceedings of the 18th International Symposium on Distributed Computing DISC'04, Amsterdam, Netherlands, October 2004.

L. Gurvits, "Algebraic, Combinatorial and Geometric Properties of Quantum Entanglement," 16th International Symposium on Mathematical Theory of Networks and Systems, Belgium, 2004.

L. Gurvits, "Combinatorial and Algorithmic Aspects of Hyperbolic Polynomials," Brooklyn Poly, October 2004.

L. Gurvits, "Combinatorial, Geometric and Algebraic Properties of Quantum Entanglement," Katholieke Universiteit Leuven, Belgium, July 2004.

L. Gurvits, "Combinatorics Hidden in Hyperbolic Polynomials and Related Topics," in Proceedings of the 16th International Symposium on Mathematical Theory of Networks and Systems, Belgium, 2004.

L. Gurvits, "Combinatorics Hidden in Hyperbolic Polynomials," Ireland National University, July 2004.

L. Gurvits, "Convex Geometry of Quantum Entanglement," SQuInT 2005, Tucson, Ariz., February 2005.

L. Gurvits, "Hyperbolic Rado Theorem," MSRI (Berkeley), March 2004.

L. Gurvits, "New Lower and Upper Bounds on the Size of Largest Multipartite Separable Ball," Institute for Quantum Computing, Waterloo, Canada, October 2004. Also given at UCLA in February 2005.

L. Gurvits, "Stability of Positive Switched Systems," ETH, Zurich, Switzerland, July 2004.

L. Gurvits, "Van der Waerden Conjecture for Mixed Discriminants," International Algebraic Conference, Moscow, Russia, 2004. Also given at the Moscow State University 250th Anniversary Conference, June 2004.

L.Gurvits, R.Shorten, O.Mason, "Preliminary Results on the Stability of Switched Positive Linear Systems," in Proceedings of the 16th International Symposium on Mathematical Theory of Networks and Systems, Belgium, 2004.

J. Hogden, R. Brewer, J. Sarracino, M. Cannon, "Blind Inversion of PINEX Data (U)," presented at JOWOG-32M, Aldermaston, U.K. (Also, an internal report, LA-CP-04-0366, Los Alamos National Laboratory.)

A. Hoisie and D. Kerbyson, "A Practical Approach to Performance Analysis and Modeling of Large-Scale Systems," full-day tutorial, IEEE/ACM SuperComputing, Pittsburgh, Pa., November 2004.

S. Jiang, F. Chen, X. Zhang, "CLOCK-Pro: An Effective Improvement of the CLOCK Replacement," in Proceedings of the 2005 USENIX Annual Technical Conference USENIX'05, Anaheim, Calif., pp. 87-100, April 2005.

C. Joslyn, "Management of Quantified Semantic Taxonomies for Biothreat Response," DIMACS Tutorial and Working Group on Order Theoretic Aspects of Epidemiology.

C. Joslyn, "Order Theoretical Knowledge Discovery," in DIMACS Workshop on Applications of Order Theory to Homeland Defense and Computer Security. (Also, a technical report, LA-UR-04-6208, Los Alamos National Laboratory.)

C. Joslyn, "Reports on Two Recent Bio-Ontology Workshops," in Proceedings of the Seventh Annual Bio-Ontologies Meeting, ISMB '04.

C. Joslyn, W. Buehring, P. Kaplan, and D. Powell, "Critical Infrastructure Protection Decision Support System (CIP/DSS): Addressing Uncertainty and Risk," technical report, LA-UR-04-6720, Los Alamos National Laboratory.

C. Joslyn, J. Cohn, S. Mniszewski, and K. Verspoor, "Order Theoretical Approaches to Automated Functional Annotation Using Bio-Ontologies," Integrated Biosciences Virtual Seminar on Genomics and Bioinformatics, virtualgenomics.org, November 2004.

C. Joslyn and S. Ferson, "Approximate Representations of Random Intervals for Hybrid Uncertainty Quantification," in Sensitivity Analysis of Model Output (SAMO04), K. Hanson and F. Hemez (editors), pp. 453-469, Los Alamos National Laboratory, <http://library.lanl.gov/cgi-bin/getdoc?event=SAMO2004&document=samo04-83.pdf>

C. Joslyn, S. Mniszewski, A. Fulmer, and G. Heaton, "The Gene Ontology Categorizer, Intelligent Systems for Molecular Biology (ISMB 2004)," a technical report, LA-UR-04-0354, August 2004.

C. Joslyn, S. Mniszewski, and K. Verspoor, "Combinatorial Knowledge Discovery for Bio-Ontology Management," Stanford Medical Informatics.

C. Joslyn, S. Mniszewski, K. Verspoor, and J. Cohn, "Improved Order Theoretical Techniques for GO Functional Annotation," poster to be presented at Intelligent Systems for Molecular Biology (ISMB 2005), March 2005.

D. Kerbyson, "Comparing Systems Using Application Performance Models," Cray Advanced Technical Workshop, Bologna, Italy, June 2004.

D. Kerbyson, "Performance Modeling of Large-Scale Systems in PERCS: A Methodology Description," IBM PERCS Project, July 2004.

D. Kerbyson, M. Lang, G. Patino, H. Amidi, "An Empirical Performance Analysis of Commodity Memories in Commodity Servers," in Proceedings of the ACM Workshop on Memory System Performance, Washington, D.C., June 2004.

*W. Klein, N. Gulbahce, H. Gould, J. Rundle, and K. Tiampo, "Structure of Fluctuations at Mean-Field and Spino Dal Critical Points," in preparation.

*Statistical Physics Days, June 24 - 26, 2004, Istanbul, Turkey. Contributed talk: "Quench depth and range of interaction effects in homogeneous and heterogeneous nucleation."

*Sixth Annual Greater Boston Area Statistical Mechanics Meeting, Oct 16, 2004, Brandeis University, MA. Contributed talk: "Quench depth and range of interaction effects in homogeneous and heterogeneous nucleation."

*APS March Meeting, Los Angeles, March 20-25, 2005. Contributed talk: "Heterogeneity in classical and non-classical nucleation."

V. Krishnamurthy, M. Faloutsos, M. Chrobak, L. Lao, J. Cui, and A. Percus, "Reducing Large Internet Topologies for Faster Simulations," in Proceedings of Networking 2005, Waterloo, Ontario, May 2-6, 2005.

M. Mathis and D. Kerbyson, "Performance and Scalability of Particle Transport Calculations," poster presentation, Department of Energy High Speed Computing Conference, Newport Beach, Ore., April 2004.

M. Mathis and D. Kerbyson, "Performance Modeling of Unstructured Mesh Particle Transport Computations," in Proceedings of the Workshop on Performance Modeling Evaluation and Optimization (PMEO), Int. Parallel and Distributed Processing Symposium (IPDPS), Santa Fe, N.M., April 2004.

K. Muske, J. Jones, and J. Howse, "Model-Based Fault Detection for Three-Way Automotive Catalyst Systems," in the Proceedings of the First IFAC Symposium on Advances in Automotive Control, Salerno, Italy, pp. 374-379, April 2004.

S. Pakin, "coNCePTuaL: A Network Correctness and Performance Testing Language," in Proceedings of the International Parallel and Distributed Processing Symposium (IPDPS 2004), Santa Fe, N.M., April 28-30, 2004. Available at <http://www.c3.lanl.gov/~pakin/papers/ipdps2004.pdf>.

S. Pakin, "Rapid Development of Application-Specific Network Performance Tests," to appear in the Proceedings of the International Conference on Computational Science (ICCS 2005), Workshop on Tools for Program Development and Analysis in Computational Science, Atlanta, Georgia, May 22-25, 2005. (Also, a technical paper, LA-UR-05-0275, Los Alamos National Laboratory.) Available at: <http://www.c3.lanl.gov/~pakin/papers/tpdacs2005.pdf>.

S. Pakin, "Reproducible Network Benchmarks with conceptual," in Proceedings of Euro-Par 2004, Pisa, Italy, August 31-September 3, 2004. (Also, a technical report, LA-UR-04-6067, Los Alamos National Laboratory.) Available at <http://www.c3.lanl.gov/~pakin/papers/europar2004.pdf>.

A. Percus, G. Istrate, and C. Moore (editors), "*Computational Complexity and Statistical Physics*," Oxford University Press, New York, 2005.

A. Percus, G. Istrate, and C. Moore, "Where Statistical Physics Meets Computation," in a forthcoming book, Computational Complexity and Statistical Physics, in production, 2005.

M. Pernice, "Performance of a Newton-Krylov-FAC Method for Equilibrium Radiation Diffusion on Locally Refined Grids," Eighth Copper Mountain Conference on Iterative Methods, April 2004.

M. Pernice, "Solution of a Streamfunction-Vorticity Formulation of Resistive Magnetohydrodynamics Using Implicit Adaptive Mesh Refinement," 16th International Conference on Domain Decomposition Methods, January 2005.

F. Petrini, "A Network Operating System for Large-Scale Parallel Machines," Emory University, Atlanta, Ga.

F. Petrini, "HPCRI (High Performance Computing Reliability Issues), in Conjunction with HPCA (High Performance Computer Architecture)," San Francisco, Calif.

F. Petrini, "System-Level Fault-Tolerance in Large-Scale Parallel Machines with Buffered Coscheduling (Keynote Speech)," Ninth IEEE Workshop on Fault-Tolerant Parallel, Distributed and Network-Centric Systems (FTPDS04), Santa Fe, N.M.

F. Petrini, K. Davis, and J. Sancho, "System-Level Fault-Tolerance in Large-Scale Parallel Machines with Buffered Coscheduling," in Ninth IEEE Workshop on Fault-Tolerant Parallel, Distributed and Network-Centric Systems (FTPDS04), Santa Fe, N.M., April 2004.

J. Sancho, F. Petrini, K. Davis, R. Gioiosa, and S. Jiang, First Workshop on System Management Tools for Large-Scale Parallel Systems, 19th International Parallel and Distributed Processing Symposium (IPDPS 2005), Denver, Colo., April 2005.

J. Sancho, A. Robles, P. Lopez, J. Flich, and J. Duato, "Performance Evaluation of COWs under Real Parallel Applications," in Proceedings of the Workshop on Communication Architecture for Clusters (CAC'03), April 22, 2003, Nice, France.

J. Sancho, A. Robles, P. Lopez, J. Flich, and J. Duato, "Routing in InfiniBand Torus Network Topologies," in Proceedings of the International Conference on Parallel Processing (ICPP'03), October 6-9, 2003, Kaohsiung, Taiwan.

E. Springer, E. Vivoni, K. Costigan, S. Mniszewski, G. Zyvoloski, P. Fasel, and G. Langhorst, "SAHRA Fine Resolution Model—Status and Needs," Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA) Fourth Annual Meeting, October 2004.

I. Steinwart, D. Hush, and C. Scovel, "Fast Rates to Bayes for Kernel Methods," Neural Information Processing Systems (reviewed conference), 2004, in press.

I. Steinwart and C. Scovel, "Anomaly Detection Is Classification," Neural Information Processing Systems (reviewed conference), 2004, in press.

I. Steinwart and C. Scovel, "When Do Support Vector Machines Learn Fast?" 16th International Symposium on Mathematical Theory of Networks and Systems 2004, invited paper with talk. Also given (with variations) at: University of Dortmund, Germany, 2004; University of Bochum, Germany, 2004; Max-Planck Institute for Biological Cybernetics, Tuebingen, Germany, 2004; AMS regional meeting, Albuquerque, N.M., 2004; PASCAL Workshop, Eindhoven, the Netherlands, 2004; 16th International Symposium on Mathematical Theory of Networks and Systems, Leuven, Belgium, 2004; LANL, 2004.

Z. Toroczkai, M. Anghel, G. Korniss, and K. Bassler, "Effects of Inter-Agent Communications on the Collective," in *Collectives and the Design of Complex Systems*, K. Tumer and D. Wolpert (editors), Springer, 2004.

K. Verspoor, J. Cohn, C. Joslyn, S. Mniszewski, A. Rechtsteiner, L. Rocha, and T. Simas, "The LANL BioCreative Task 2 Submission," poster at Intelligent Systems for Molecular Biology (ISMB 2004), August 2004.

K. Verspoor, J. Cohn, C. Joslyn, S. Mniszewski, A. Rechtsteiner, L. Rocha, and T. Simas, "Protein Annotation as Term Categorization in the Gene Ontology," Biocreative Workshop. (Also, a technical report, LA-UR-04-1460, Los Alamos National Laboratory.)

K. Verspoor, J. Cohn, S. Mniszewski, and C. Joslyn, "Nearest Neighbor Categorization for CASP Function Prediction," poster to be presented at Intelligent Systems for Molecular Biology (ISMB 2005), March 2005.

K. Verspoor, J. Cohn, S. Mniszewski, and C. Joslyn, "Nearest Neighborhood Categorization for Function Prediction," in the Proceedings of the Fifth Community-Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction (CASP 05), in press.

K. Verspoor, J. Cohn, S. Mniszewski, and C. Joslyn, "Nearest Neighbor Categorization for Function Prediction," in Proceedings of the Sixth Community-Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction," Gaeta, Italy. December 4-8. (Also, a technical report, LA-UR-04-7477, Los Alamos National Laboratory.)

T. Warnock, "A Shape Metric Based on the Line Scan Transform," a talk at the Nuclear Explosives Code Developers Conference (NECDC).

T. Warnock, "Statistical Methods for Analysis and Anomaly Detection in Large Hydrocode Datasets," a talk at the Nuclear Explosives Code Developers Conference (NECDC).

Media

K. Patch, "Agent Model Yields Leadership," *Technology Research News*, September 22/29, 2004, text available at:
www.trnmag.com/Stories/2004/092204/Agent_model_yields_leadership_092204.html

Research in Progress

S. Pakin, "The Design and Implementation of a Domain-Specific Language for Network Performance Testing," submitted to the 14th International Conference on Parallel Architectures and Compilation Techniques (PACT-2005).

L. Gurvits, a classical black-box approach to search problems with the same complexity bounds as in Lov Grover's quantum algorithm, 2005.

L. Gurvits, "On the Complexity of Mixed Discriminants and Related Problems," 2005.

L. Gurvits and H. Barnum, "Further Results on the Multipartite Separable Ball," see <http://xxx.lanl.gov/abs/quant-ph/0409095>. 2004.

L. Gurvits and H. Barnum, "Revisiting Separability of 2x2 Quantum Systems," a paper dealing with the quaternionic approach to quantum separability, 2005.

L. Gurvits and A. Samorodnitsky, "A Note on Common Quadratics Lyapunov Functions for Linear Inclusions: Exact Results and Open Problems," technical report, LA-UR-05-1937, Los Alamos National Laboratory.

B. Philip and M. Pernice, "Performance of FAC Preconditioners for Multi-Material Equilibrium Radiation Diffusion on Adaptively Refined Grids."

B. Philip, M. Pernice, and L. Chacon, "Solution of Reduced Resistive Magnetohydrodynamics Using Implicit Adaptive Mesh Refinement."

Software

S. Pakin released coNCePTuaL on August 24, 2004, LA-CC-03-099. Available from <http://conceptual.sourceforge.net/>.

Awards

Several staff members in CCS-3 received the Defense Programs Award of Excellence for work done by the ASCI Lightning Integration Team, October 2004.

Computational Biology (CB) Team

L. Bettencourt, A. Cintron-Arias, D. Kaiser, and C. Castillo-Chavez, "The Power of a Good Idea: Quantitative Modeling of the Spread of Ideas from Epidemiological Models," submitted to *PRE*.

L. Bettencourt, J. Lobo, and D. Strumsky, "Innovation in the City: Increasing Returns to Scale in Metropolitan Patenting," submitted to *Research Policy*.

M. Dunlop and M. Wall, "Robustness in Gene Circuits: Clustering of Functional Responses," *Proceedings of the 24th American Control Conference*, in press.

L. Gomes, R. Almeida, L. Bettencourt, V. Almeida, and J. Almeida, "Comparative Graph Theoretical Characterization of Networks of Spam and Legitimate E-Mail," submitted to CEAS05 conference.

L. Gomes, R. Almeida, L. Bettencourt, V. Almeida, and J. Almeida, "Improving Spam Detection Based on Structural Similarity," submitted to *ACM Transactions on Information and System Security (TISSEC)*.

D. Ming and M. Wall, "Quantifying Allosteric Effects in Proteins," *Proteins*, published online, April 8, 2005.

M. Wall, M. Dunlop, and W. Hlavacek, "Multiple Functions of a Feed-Forward-Loop Gene Circuit," *J Mol Biol*, in press.

Transport Methods (CCS-4)

D. Carrington, D. Pepper, "Indoor Air Pollution Modeling," Chapter 14 of *Air Quality Modeling, Theories, Methodologies, Computational Techniques, Available Databases and Software*, Vol. II Advanced Topics, Zannetti, P. (editor). (Also a technical report, LA-UR-04-2508, Los Alamos National Laboratory.)

D. Carrington, S. Turner, "Explicit Correction for Material Motion in Radiative Transfer," Los Alamos National Laboratory/CCS Memorandum, CCS-4:05-04, 2005.

D. Carrington, S. Turner, "Verification of Material Motion Correction for the Radiative Transfer Equations," Los Alamos National Laboratory, LA-UR-04-7895, 2004

D. Carrington, V. Mousseau, "Preconditioning and Solver Optimization Ideas for Radiative Transfer," Los Alamos National Laboratory, LA-UR-05-1444, 2005. (Also, ASME Heat Summer Transfer Conference 2005, paper #HT2005-72040.)

D. Carrington, V. Mousseau, "Preconditioning and Solver Optimization for Radiative Transfer," Los Alamos National Laboratory, LA-UR-04-1889, 2004. (Also presented at the Eight Copper Mountain Conference on Iterative Methods, March 28-April 2, 2004.)

J. Densmore, "An Improved Method for Treating Monte Carlo-Diffusion Interfaces," *Trans. Am. Nucl. Soc.*, 91, 139 (2004).

J. Densmore and E. Larsen, "Asymptotic Equilibrium Diffusion Analysis of Time-Dependent Monte Carlo Methods for Grey Radiative Transfer," *J. Comp. Phys.*, 199, 175, 2004.

J. Densmore, T. Urbatsch, T. Evans, and M. Buksas, "Discrete Diffusion Monte Carlo for Grey Implicit Monte Carlo Simulations," in the *Proceedings of Int. Top. Mtg. Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Avignon, France, September 12-15, 2005, submitted.

T. Evans, J. Densmore, and T. Urbatsch, "Equilibrium-Diffusion Material Motion Correction for Wedgehog," CCS-4:05-06(U), January 19, 2005.

A. Hungerford, J. Densmore, and M. Buksas, "Compton Scattering in Implicit Monte Carlo," CCS-4:05-14(U), March 17, 2005.

J. Morel and J. Densmore, "A Two-Component Equilibrium-Diffusion Limit," *Ann. Nucl. Energy*, 31, 2049 (2004).

J. Morel and J. Warsa, "An SN Spatial Discretization Scheme for Tetrahedral Meshes," *Nuclear Science and Engineering*, submitted in 2004, accepted for publication in 2005.

S. Mosher and F. Rahnema, "A Decoupled Finite Element Heterogeneous Coarse Mesh Transport Method," *Transactions of the American Nuclear Society*, Vol. 92, June 2005.

R. Ward, R. Baker, and J. Morel, "A Diffusion Synthetic Acceleration Method for Block Adaptive Mesh Refinement," to be published in *Nucl. Sci and Eng*.

R. Ward, R. Baker, and J. Morel, "A Diffusion Synthetic Acceleration Method for Block Adaptive Mesh Refinement," submitted to *Nucl. Sci and Eng*.

R. Ward and D. Steiner, "The EPQ Code System for Simulating the Thermal Response of Plasma Facing Components to High Energy Electron Impact," *Fus. Sci. and Tech.*, Vol. 45, n 4, 529-548, 2004.

J. Warsa, "Preconditioning a Parallel, Inexact Block-Jacobi Splitting of the SN Algorithm," accepted for presentation at the 2005 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Scientific and Industrial Applications, May 19-21, Emory University, Atlanta, Georgia.

Discrete Simulation Science (CCS-DSS)

H. Balakrishnan, C. Barrett, V. Kumar, M. Marathe, S. Thite, "The Distance-2 Matching Problem and Its Relationship to the MAC-Layer Capacity of Ad Hoc Networks," *IEEE Journal on Selected Areas in Communication*, 22(6), pp 1069-1079, 2004.

C. Barrett, M. Drozda, D. Engelhart, V. Kumar, M. Marathe, M. Morin, S. Ravi, and J. Smith, "Understanding Protocol Performance and Robustness of Ad Hoc Networks through Structural Analysis," *IEEE International Conference on Wireless and Mobile Computing, Networking and Communications (WiMob)*, 2005.

C. Barrett, S. Eidenbenz, L. Kroc, M. Marathe, and J. Smith, "Parametric Probabilistic Sensor Network Routing," *Mobile Networking (MONET) Special Issue on WSNA 2003*, 2005.

C. Barrett, S. Eidenbenz, L. Kroc, M. Marathe, and J. Smith, "Scenario-Dependent Routing in Mobile Wireless Networks," in the *Proceedings of ACM Symposium on Applied Computing 2005*.

M. Cieliebak and S. Eidenbenz, "Measurement Errors Make the Partial Digest Problem NP-Hard," in the *Proceedings of Latin American Theoretical Informatics 2004*.

M. Cieliebak, S. Eidenbenz, and P. Penna, "Partial Digest Is Hard to Solve for Erroneous Input Data," *Theoretical Computer Science*, Elsevier Science, 2004.

M. Cieliebak, S. Eidenbenz, and G. Woeginger, "Complexity and Approximability of Double Digest," *Journal of Bioinformatics and Computational Biology*, Vol. 3, No. 2, pp. 1-17, 2005.

- S. Eidenbenz, V. Kumar, and S. Züst, "Equilibria in Topology Control Games for Ad Hoc Networks," *Special Issue of ACM Baltzer Mobile Networks and Applications (MONET)*, 2004.
- S. Eidenbenz, G. Resta, P. Santi, "COMMIT: A Sender-Centric Truthful and Energy-Efficient Routing Protocol for Ad Hoc Networks," in the *Proceedings of IEEE WMAN 2005*.
- S. Eubank, H. Guclu, V. Kumar, M. Marathe, A. Srinivasan, Z. Toroczkai, and N. Wang, "Modeling Disease Outbreaks in Realistic Urban Social Networks," *Nature*, 429, 180-184 (2004).
- S. Eubank, V. Kumar, M. Marathe, A. Srinivasan, and N. Wang, "Structural and Algorithmic Aspects of Massive Social Networks," *ACM Symposium on Discrete Algorithms (SODA)*, 2004.
- A. Hansson and T. Aulin, "Generalized APP Detection for Communication over Unknown ISI Channels," *IEEE Transactions on Communications*, 2004.
- A. Hansson and M. Nassr, "On-Line Wavelet Compression with Dynamic Resolution," in the *Proceedings of the 38th Annual Conference on Information Sciences and Systems, Princeton*, 2004.
- G. Istrate, "On the Satisfiability of Random k-Horn Formulas, in Graphs, Morphisms and Statistical Physics," *AMS-DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, pp. 113-136, 2004.
- V. Kumar, M. Marathe, S. Parthasarathy, and A. Srinivasan, "Algorithmic Aspects of Capacity in Wireless Networks," *ACM SIGMETRICS*, 2005.
- V. Anil Kumar, M. Marathe, S. Parthasarathy, and A. Srinivasan, "End-to-End Packet Scheduling in Ad Hoc Networks," *ACM Symposium on Discrete Algorithms (SODA)*, 2004.
- V. Kumar, M. Marathe, S. Parthasarathy, A. Srinivasan, and S. Züst, "Provable Algorithms for Parallel Sweep Scheduling on Unstructured Meshes," *International Parallel and Distributed Processing Symposium (IPDPS)*, 2005.
- H. Mortveit and C. Reidys, "Neutral Evolution and Mutation Rates of Sequential Dynamical Systems," *Advances in Complex Systems*, 2004.
- H. Mortveit and C. Reidys, "Reduction of Discrete Dynamical Systems," *Advances in Complex Systems*, Vol. 7, No. 1, 1-20, 2004.
- H. Mortveit and C. Reidys, "Reduction of Discrete Dynamical Systems over Graphs,"

SIAM Conference on Discrete Mathematics, 2004.

H. Mortveit and C. Reidys, "Sequential Dynamical Systems: A Mathematical Framework for Computer Simulations," *Conference of Mathematical Theory of Networks and Systems*, 2004.

C. Reidys, "Distance-2-Matchings of Random Graphs," *Annals of Combinatorics*, 8:93-101, 2004.

C Reidys, "On a Certain Class of Morphisms of Sequential Dynamical Systems," *Discrete Mathematics*, 2005.

J. Tripp, A. Hansson, H. Mortveit, and M. Gokhale, "Metropolitan Road Traffic Simulation on FPGAs," *IEEE Symposium on Field-Programmable Custom Computing Machines*, 2005.

J. Tripp, A. Hansson, H. Mortveit, and M. Gokhale, "Road Traffic Simulation on the Cray XD1," *47th Cray User Group Conference*, 2005.

J. Tripp, H. Mortveit, M. Nassr, A. Hansson, and M. Gokhale, "Acceleration of Traffic Simulation on Reconfigurable Hardware," *Military and Aerospace Applications of Programmable Devices and Technologies International Conference*, 2004.